Last update: 27 September 2024

# 原著論文/著書リスト

## 原著論文/全て査読有(A185 以下が採録決定済/A191 以下が arXiv 済)

* A191; " Topological data analysis for revealing structural origin of density anomalies in silica glass",
(***)

A. Tirelli, K. Nakano,
arXiv: 2208.06378 (2022)

* A190; " High-$T_c$ superconductivity of clathrate $Y_3EuH_{24}$",
(クラスレート構造イットリウム・ユーロピウム水素化物の高温超伝導)

A. Ghaffar, P. Song, K. Nakano, K. Hongo, R. Maezono,
arXiv:2205.05906 (2022)

* A189; " Quantum phase diagram of high-pressure hydrogen",
(第一原理量子モンテカルロ法を利用した高圧水素の量子相図研究)

Lorenzo Monacelli, Michele Casula, Kosuke Nakano, Sandro Sorella, Francesco Mauri,
arXiv:2202.05740 (2022)

* A188; "High-$T_c$ ternary metal hydrides, $YKH_{12}$ and $LaKH_{12}$, discovered by machine learning",
(機械学習的探索で発見された高温超伝導 3 元水素化物)

P. Song, H. Zhufeng, P. Baptista de Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono,
arXiv:2103.00193 (2021)

* A187; "First Principles Calculations of Superconducting Critical Temperature of $ThCr_2Si_2$-Publisher Structure",
($ThCr_2Si_2$ 型化合物の超伝導転移温度に関するハイスループットスクリーニング)

G.S. Sinaga, K. Utimula, K. Nakano, K. Hongo, R. Maezono,
(in preparation for J. Phys. Chem. C (2022/IF= 3.7))
arxiv.org/abs/1911.10716

*A186; "Importance of vdW and long-range exchange interactions to DFT-predicted docking energies between plumbagin and cyclodextrins"

(シクロデキストリンのホストゲスト結合予見における電子相関)

T. Ichibha, O. Srihakulung, G. Chao, A. T. Hanindriyo, L. Lawtrakul, K. Hongo, R. Maezono,
arXiv:1904.02503(2019)

* A185; "Using reinforcement learning to autonomously identify the source of errors for agents in group missions",

(原因系を効率よく切り分ける検証行動計画を自動的に策定する強化学習)

K. Utimula*, K-T. Hayaschi, T. J. Bihl, K. Nakano, K. Hongo, R. Maezono,
**Front. Control Eng.**, in press, (2024) [Q2-journal]
DOI : 10.3389/fcteg.2024.1402621

* A184; "Solid-liquid phase boundary of oxide solid solutions using neural network potentials",

(***)

K. Hyodo, K. Hongo, T. Ichibha, R. Maezono*,
**J. Alloys Compd.**, in press, (2024) [Q1-journal]
DOI : 10.1016/j.jallcom.2024.176227

* A183; "Structural predictions and phonon-mediated superconductivity in platinum hydride under low pressure: Insight from first-principles calculations",

(***)

P. Tsuppayakorn-aek, P. Song, W. Sukmas, R. Maezono, T. Bovornratanaraks,
**Comput. Mater. Sci.**, 244, 113265(2024) [Q1-journal]
DOI : 10.1016/j.commatsci.2024.113265

* A182; "Ca substitution effects on structure transformation and physical properties of (Eu,Ca)$FeAs_2$ co-doped with La and Co",

(***)

S. P. K. Naik*, S. Alberto, K. Kataoka, Y. Gotoh, T. Ichibha, K. Hongo, R. Maezono, T. Nishio, H. Ogino*,
**Ceram. Int.**, 50, 40830-40838, (2024) [Q1-journal]
DOI : 10.1016/j.ceramint.2024.07.374

* A181; "Thermal Decomposition of Oxygen-containing $Ta_3N_5$",

(タンタル窒化物への酸素ドープに関する状態図解析)

N. Moharana, C. Ghosh, A. Dasgupta, R. Maezono, S. Sarma, Ravi Kumar, K.C.Hari Kumar,
**J. Am. Ceram. Soc.**, 107, 6342-6352(2024) [Q1-journal]
DOI : 10.1111/jace.19869

* A180; "Substitutional Doping Strategies for Fermi Level Depinning and Enhanced Interface Quality in WS2-Metal Contacts",
(ドープした遷移金属ダイカルゴゲナイトの界面に関する第一原理解析)

A. Ghaffar, N.R. Mohapatra, K. Hongo, and R. Maezono,
**ACS Appl. Electron. Mater.**, 6, 4587-4600 (2024) [Q1-journal]
DOI : 10.1021/acsaelm.4c00609

* A179; "Key Role of Metal-to-Metal Charge Transfer Transition between $Mo^{6+}$ and $Bi^{3+}$ for Enhancement in NIR Luminescence of $Gd_2MoO_6$:Bi,Yb Nanophosphor",
(ナノ蛍光体の発光を増強させる金属イオン間の電荷移動)

T. Hangai, *T. Hasegawa, J. Xu, T. Nakanishi, T. Takeda, K. Nakano, K. Hongo, R. Maezono, T. Goto, Y. Sato, A. Okawa, S. Yin,
**J. Phys. Chem. C.** 128, 3351-3360 (2024) [Q1-journal]
DOI : 10.1021/acs.jpcc.3c07501

* A178; "Single crystal growth and physical properties of La, Co doped (Eu,Ca)$FeAs_2$",
(新規鉄系化合物単結晶の基礎物性解析)

*S. P. K. Naik, S. Alberto, K. Kataoka, Y. Gotoh, T. Ichibha, K. Hongo, R. Maezono, T. Nishio, *H. Ogino,
**J. Cryst. Growth.** 628, 127547 (2024) [Q2-journal]
DOI : 10.1016/j.jcrysgro.2023.127547

* A177; "Multi-emission of $Ce^{3+}$ from Single Crystallographic Site Induced by Disordering of Ions",
(秩序の乱れに起因した $Ce^{3+}$からの発光バリエーション)

T. Yasunaga, *M. Kobayashi, K. Oqmhula, H. Qi, T. Ichibha, K. Hongo, S. Yamamoto, R. Maezono, M. Mitsuishi, M. Osada, *H. Kato, M. Kakihana,
**Inorg. Chem.** 63, 1288－1295 (2024) [Q1-journal]
DOI : 10.1021/acs.inorgchem.3c03789

* A176; "Locality Error Free Effective Core Potentials for 3d Transition Metal Elements Developed for the Diffusion Monte Carlo Method",
(量子拡散モンテカルロ法用途の有効各電荷の開発--3d 遷移金属における局所近似誤差問題の解決)

*T. Ichibha, Y. Nikaido, C. M Bennett, J. T Krogel, K. Hongo, R. Maezono, *F. A Reboredo,
**J. Chem. Phys.** 159 164114 (2023) [Q1-journal]
DOI : 10.1063/5.0175381

* A175; "$(La,Th)H_{10}$: Potential high-$T_c$ (242 K) superconductors Stabilized Thermodynamically below 200 GPa",
(高圧下におけるランタン・トリウム水素化物の高温超伝導)

*P. Song, A. P. Durajski, Z. Hou, A. Ghaffar, R. Dahule, R. Szcze̜śniak, K. Hongo, R. Maezono,
**J. Phys. Chem. C .** 128 2656–2665 (2024) [Q1-journal]
DOI : 10.1021/acs.jpcc.3c07213

* A174; "First-Principles Investigation of Stability and Superconductivity in Ternary Yttrium − Praseodymium Hydrides under High Pressure",
(遺伝的アルゴリズムを用いた高圧下の Y-Pr 水素化物における超伝導と合成安定性の予見)

*K. S. Qin, *P. Song, *K. Hongo, *R. Maezono,
**J. Phys. Chem. C** 127 21242-21249 (2023) [Q1-journal]
DOI : 10.1021/acs.jpcc.3c02968

* A173; "Structure, optical, and electrical properties of layered oxychalcogenide $Sr_2ZnCu_2(S_{1-x}Se_x)_2O_2$ ($0 \le x \le 1$) compounds",
(層状カルコゲナイト酸化物の構造と光学物性、電子物性)

T. Kato, Y. Iwasa, S. Pavan K. Naik, S. Ishida, Y. Higashi, I. Hase, T. Nishio, K. Hongo, R. Maezono, *H. Ogino,
**Mater. Res. Express** 10, 095904 (2023) [Q2-journal]
DOI : 10.1088/2053-1591/acf54d

* A172; "Recognition of spatial finiteness in meniscus splitting based on evaporative interface fluctuations",
(***)

L. Wu, I. Saitoh, K. Hongo, *K. Okeyoshi,
**Adv. Mater. Interfaces** 2300510, 1-8 (2023) [Q1-journal]
DOI : 10.1002/admi.202300510

* A171; "Stiffer Bonding of Armchair Edge in Single-Layer Molybdenum Disulfide Nanoribbons",
(***)

C. Liu, K. Hongo, R. Maezono, *J. Zhang, *Y. Oshima,
**ACS Appl. Mater. Interfaces** 10, 2303477 (2023) [Q1-journal]
DOI : 10.1002/advs.202303477

* A170; "Biophysical properties of fibril structure of the toxic conformer of amyloid-β42: characterization by atomic force microscopy and molecular docking",
(毒性型アミロイドベータのフィブリル構造に関するドッキングシミュレーションと原子力顕微鏡観測)

R. Biyani, K. Hirata, K. Oghmhula, A. Yurtsever, K. Hongo, R. Maezono, M. Takagi, *T. Fukuma, *M. Biyani,
**ACS Appl. Mater. Interfaces,** 15, 27789–27800 (2023) [Q1-journal]
DOI : 10.1021/acsami.3c06460

* A169; "Existence of La-site antisite defects in $LaMO_3$ (M = Mn, Fe, and Co) predicted with many-body diffusion quantum Monte Carlo",
(LaMO3 型ペロブスカイト中アンチサイト欠陥 -- 量子拡散モンテカルロ法による存在予見)

T. Ichibha, S. Yoon, J. M. Ok, M. Yoon, H. N. Lee, F. A. Reboredo,
**Sci. Rep.,** 13 6703 (2023) [Q1-journal]
DOI : 10.1038/s41598-023-33578-1

* A168; "High-pressure BaCN2 phases explored by genetic algorithm",
(遺伝アルゴリズムを用いた金属カルボジイミド結晶の構造探索)

P. Song, M. Khawaguch, Y. Masubuchi, K. Oqmhula, K. Nakano, R. Maezono, K. Hongo,
**Comput. Mater. Sci.** 226 112202 (2023) [Q1-journal]
DOI : 10.1016/j.commatsci.2023.112202

* A167; "Evolutionary Algorithm Directed Synthesis of Mixed Anion Compounds LaF2X (X = Br, I) and LaFI2.",
(遺伝的アルゴリズムを援用したフッ化物複合アニオン物質の合成)

D. Kato, P. Song, H. Taguro, C. Tassel, H. Ubukata, K. Miyazaki, T. Abe, K. Nakano, T. Ichibha, K. Hongo, *R. Maezono, *H. Kageyama,,
**Angew. Chem. Int. Ed.** e202301416 (2023) [Q1-journal]
DOI : 10.1002/anie.202301416

* A166; "Towards chemical accuracy using the Jastrow correlated antisymmetrized geminal power ansatz",
(ジェミナル型多体波動関数で化学的精度を実現する電子状態計算)

A. Raghav, R. Maezono, K. Hongo, S. Sorella, K. Nakano,
**J. Chem. Theory Comput.** 19, 2222-2229 (2023) [Q1-journal]
DOI : 10.1021/acs.jctc.2c01141

* A165; "Thermodynamic Understanding of Impurity Phase Segregation in a PdCrO2/CuCrO2 Heterostructure",
(LaMO3 型ペロブスカイト中アンチサイト欠陥 -- 量子拡散モンテカルロ法による存在予見)

T. Ichibha, S. Yoon, J. M. Ok, M. Yoon, H. N. Lee, F. A. Reboredo,
**Advanced Physics Research** (2023) ,
DOI : 10.1002/apxr.202200080

* A164; "First-Principles-Based Insight into Electrochemical Reactivity in A Cobalt-Carbonate-Hydrate Pseudocapacitor",
(電気化学キャパシタ材料の蓄電特性をスーパーコンピュータを用いたシミュレーションで解明)

K. Oqmhula, T. Toma, R. Maezono, K. Hongo,
**ACS Omega** 8, 6743-6752 (2023) [Q1-journal]
DOI : 10.1021/acsomega.2c07362

* A163; "Mechanistic insights and importance of hydrophobicity in cationic polymers for cancer therapy",
(抗ガン高分子の分子設計指針に新たな光～カチオン性と疎水性の相乗効果で高い細胞障害性が発現～)

N. Kumar, K. Oqmhula, K. Hongo, K. Takagi, S. Yusa, R. Rajan, K. Matsumura,
**J. Mater. Chem. B.** 11, 1456-1468 (2023) [Q1-journal]
DOI : 10.1039/D2TB02059A

* A162; "Order–disorder competition in equiatomic 3d–transition–metal quaternary alloys: Phase stability and electronic structure",
(3d 遷移金属等組成 4 元系合金における秩序-無秩序競合：相安定性と電子状態)

H. Mizuseki, R. Sahara, K. Hongo,
**Sci. Technol. Adv. Mater.** 3, 2153632 (2023) [Q1-journal]
DOI : 10.1080/27660400.2022.2153632

* A161; "Electronic and magnetic properties of pure and Cu doped non-polar ZnO($10\bar{1}0$) surfaces",
(Cu をドープした ZnO 表面の電気的磁気的性質に関する第一原理解析)

E. Irandegani, R. Maezono, M. Abbasnejad,
**J. Appl. Phys.** 132 173903 (2022) [Q2-journal]
DOI : 10.1063/5.0106799

* A160; "Feature space of XRD patterns constructed by auto-encorder",
(オートエンコーダによって構成された XRD パターンの特徴量空間)

K. Utimula, M. Yano, H. Kimoto, K. Hongo, K. Nakano, R. Maezono,
**Adv. Theory Simul.** 2200613, (2022) [Q1-journal]
DOI : 10.1002/adts.202200613

* A159; " Potential high-$T_c$ superconductivity in $YCeH_{20}$ and $LaCeH_{20}$ under pressure",
(Ce 系水素化物の高圧化超伝導)

P. Song, Z. Hou, K. Nakano, K. Hongo, R. Maezono,
**Mater. Today Phys.**, 28 100873 (2022) [Q1-journal]
DOI : 10.1016/j.mtphys.2022.100873

* A158; "Anionic ordering in $Pb_2Ti_4O_9F_2$ revisited by nuclear magnetic resonance and density functional theory",
(鉛酸フッ化物のローンペアで安定化されるアニオン秩序配列)

K. Oka, T. Ichibha, D. Kato, M. Iwasaki, N. Noma, K. Hongo, R. Maezono, F. A. Reboredo,
**Dalton Trans. 51, 15361-15369**, (2022) [Q1-journal]
DOI : 10.1039/D2DT00839D

* A157; "Ab-initio-based Interface Modeling and Statistical Analysis for Estimate of the Water Contact Angle on a Metallic Cu(111) Surface",
(第一原理計算による界面モデリング:金属表面に対する接触角評価)

T. Murono, K. Hongo, K. Nakano, R. Maezono,
**Surf. Interfaces** 34, 102342 (2022) [Q1-journal]
DOI : 10.1016/j.surfin.2022.102342

* A156; " Electronic structure and effective mass analysis of doped $TiO_2$ (anatase) systems using DFT+$U$",
(ドープしたチタン酸化物の DFT+U 電子状態計算と有効質量解析)

A. Raghav, K. Hongo, R. Maezono, E. Panda,
**Comput. Mater. Sci.** 214, 111714(2022) [Q1-journal]
DOI : 10.1016/j.commatsci.2022.111714

* A155; "Ab initio molecular dynamics simulation of structural and elastic properties of SiO2-P2O5-Al2O3 glass",
(ガラス材料の力学特性に関する第一原理分子動力学解析)

Y. Qian, B. Song, J. Jin, G. I. Prayogo, K. Utimula, K. Nakano, R. Maezono, K. Hongo, G. Zhao,
**J. Am. Ceram. Soc.** 105, 6604-6615(2022) [Q1-journal]
DOI : 10.1111/jace.18614

* A154; "High pressure hydrogen by machine learning and quantum Monte Carlo",
(厳密な電子状態計算 × 機械学習ポテンシャル:高圧水素における液体-液体相転移の研究)

A. Tirelli, G. Tenti, K. Nakano, S. Sorella,
**Phys. Rev. B** 106, L041105 (2022) [Q1-journal]
DOI : 10.1103/PhysRevB.106.L041105

* A153; " SHRY: Application of canonical augmentation to the atomic substitution problem",
(SHRY:正準強化法の原子置換問題への応用)

I. Prayogo, A. Tirelli, K. Utimula, K. Hongo, R. Maezono, K. Nakano,
**J. Chem. Inf. Model** 62, 2909-2915 (2022) [Q1-journal]
DOI : 10.1021/acs.jcim.2c00389

* A152; " High pressure behavior of tetragonal barium carbodiimide, BaNCN",
(カルボジイミド無機化合物の結晶構造の X 線回折および密度汎関数法による解析)

Y. Masubuchi, S. Miyazaki, P. Song, T. Yamamoto, K. Nakano, K. Hongo, R. Maezono,
**J. Alloys Compd.** 918, 165632 (2022) [Q1-journal]
10.1016/j.jallcom.2022.165632

* A151; " Computational design to suppress thermal runaway of Li-ion batteries via atomic substitutions to cathode materials",
(元素置換による LiNiO2 の熱安定化)リチウムイオン電池の熱暴走を抑制するナノレベル材料設計)

Y. Yoshimoto, T. Toma, K. Hongo, K. Nakano, R. Maezono,
**ACS Appl. Mater. Interfaces** 14, 23355-23363 (2022) [Q1-journal]
DOI : 10.1021/acsami.2c01607

* A150; "Impact of Surface Faceting on Gas Sensing Selectivity of NiO: Revealing the Adsorption Sites of Organic Vapors on the {111} Facet",
(NiO(111)面のガス吸着選択性)

A. Hermawan, A. T. Hanindriyo, K. Hongo, R. Maezono, S. Yin,
**J. Phys. Chem. C.** 126, 8037–8046 (2022) [Q1-journal]
DOI : 10.1021/acs.jpcc.2c00092

* A149; " Lattice Dynamics in the NASICON NaZr2(PO4)3 Solid Electrolyte from Temperature-Dependent Neutron Diffraction, NMR, and Ab Initio Computational Studies",
(***)

E. E. Morgan, H. A. Evans, K. Pilar, C. M. Brown, R. J. Clément, R. Maezono, R. Seshadri, *B. Monserrat, *A. K. Cheetham,
**Chem. Mater.,** 34, 4029-4038 (2022) [Q1-journal]
DOI : 10.1021/acs.chemmater.2c00212

* A148; " Making the most of data: Quantum Monte Carlo Post-Analysis Revisited",
(マルコフ鎖量子モンテカルロ法の効率的なリブロッキング処理)

T. Ichibha, V. A. Neufeld, K. Hongo, R. Maezono, A.J.W. Thom,
**Phys.Rev.E** 105, 045313 (2022) [Q1-journal]
DOI : 10.1103/PhysRevE.105.045313

* A147; " Stepwise copolymerization of polybenzimidazole for a low dielectric constant and ultrahigh heat resistance",
(特異な熱電効率を示すバイオポリベンザゾールの物質設計)

X. Zhong, A. Nag, J. Zhou, K. Takada, F. A. A. Yusof, T. Mitsumata, K. Oqmhula, K. Hongo, R. Maezono, T. Kaneko,
**RSC Adv.** 12, 11885 (2022) [Q1-journal]
DOI : 10.1039/D2RA01488B

* A146; " Diffusion Monte Carlo Study on Relative Stabilities of Boron Nitride Polymorphs",
(拡散量子モンテカルロ法に基づく窒化ホウ素結晶多形の相対的安定性の研究)

Y. Nikaido, T. Ichibha, K. Hongo, F. A. Reboredo, K.C. H. Kumar , P. Mahadevan, R. Maezono, K. Nakano,
**J. Phys. Chem. C.** 126, 6000-6007 (2022) [Q1-journal]
DOI : 10.1021/acs.jpcc.1c10943

* A145; " Anomalies in the bulk and surface electronic properties in SnS: Effect of native defects",
(太陽電池材料・硫化スズの電子物性における格子欠陥の影響)

Rohit Dahule, Chetan C. Singh, Kenta Hongo, Ryo Maezonob, Emila Panda,
**J. Mater. Chem. C** 10, 5514-5525 (2022) [Q1-journal]
DOI : 10.1039/D1TC04738H

* A144; "High-pressure Mg-Sc-H phase diagram and its superconductivity from first-principles calculations",
(Mg-Sc-H 化合物系における高圧構造の安定性と高温超伝導発現機構の系統的研究)

P. Song, Z. Hou, P. B. d. Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono,
**J. Phys. Chem. C.** 126, 2747–2755 (2022) [Q1-journal]
**DOI : 10.1021/acs.jpcc.1c08743**

* A143; "Diffusion Monte Carlo evaluation of Disiloxane linearization barrier",
(スーパーコンピュータを活用して分子構造シミュレーション上の有名な難問を解決)

A. T. Hanindriyo, A. K. S. Yadav, T. Ichibha, R. Maezono, K. Nakano, K. Hongo,
**Phys. Chem. Chem. Phys.** 24, 3761-3769 (2022) [Q1-journal]
**DOI : 10.1039/D1CP01471D**

* A142; "Space-warp coordinate transformation for efficient ionic force calculations in quantum Monte Carlo",
(物質中の原子に働く力を高精度かつ高速に評価する手法を開発)

K. Nakano, A. Raghav, S. Sorella,
**J. Chem. Phys.** 156, 034101 (2021) [Q1-journal]
**DOI : 10.1063/5.0076302**

* A141; "The systematic study on the stability and superconductivity of Y-Mg-H compounds under high pressure",
(Y-Mg 系三元水素化物高温超伝導体の構造安定性に関する系統的研究)

P. Song, Z. Hou, P. B. d. Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono,
**Adv. Theory Simul.** 2100364 (2021) [Q1-journal]
**DOI : 10.1002/adts.202100364**

* A140; "Candidate Structure of the H2-PRE Phase of Solid Hydrogen",
(水素結晶の高圧相に見いだされた新たな結晶相)

T. Ichibha, Y. Zhang, K. Hongo, R. Maezono, F. A. Reboredo,
**Phys. Rev. B** 104, 214111 (2021) [Q1-journal]
**DOI : 10.1103/PhysRevB.104.214111**

* A139; "High-$T_c$ superconducting hydrides formed by the cage structures $LaH_{24}$ and $YH_{24}$ as basic blocks"
(ケージ構造 $LaH_{24}$, $YH_{24}$ を基本ブロックとした超伝導水素化物)

P. Song, H. Zhufeng, P. Baptista de Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono,
**Chem. Mater.** 33, 9501-9507 (2021) [Q1-journal]
**DOI : 10.1021/acs.chemmater.1c02371**

* A138; "Site-selective $Eu^{3+}$ Luminescence in Monoclinic Phase of $YSiO_2N$"
(イットリウム蛍光体における発光増強)

Y. Kitagawa, J. Ueda, K. Fujii, M. Yashima, S. Funahashi, T. Nakanishi, N. Takashi, T. Hirosaki, K. Hongo, R. Maezono, S. Tanabe,
**Chem. Mater.** 33, 8873–8885 (2021) [Q1-journal]
**DOI : 10.1021/acs.chemmater.1c03139**

* A137; "Importance of van der Waals interactions in hydrogen adsorption on a silicon-carbide nanotube revisited with vdW-DFT and quantum Monte Carlo"
(SiC ナノチューブへの水素分子の吸着)

G. I. Prayogo, H. Shin, A. Benali, R. Maezono, K. Hongo,
**ACS Omega** 6, 24630–24636 (2021) [Q1-journal]
**DOI : 10.1021/acsomega.1c03318**

* A136; "Peculiar Atomic Bond Nature in Platinum Monatomic Chains"
(1 次元単原子鎖の力学的強度に関する解析)

J. Zhang, K. Ishizuka, M. Tomitori, T. Arai, K. Hongo, R. Maezono, E. Tosatti, Y. Oshima,
**Nano Lett.** 21, 3922-3928 (2021) [Q1-journal]
**DOI : 10.1021/acs.nanolett.1c00564**

* A135; "High-throughput evaluation of discharge profile of LiNi1－xXxO2 by ab initio calculations"
(LiNi1－xXxO2 における放電プロファイルの網羅的な 第一原理計算)

S. Yoshio, K. Hongo, K. Nakano, R. Maezono,
**J. Phys. Chem. C.** 125, 14517–14524 (2021) [Q1-journal]
**DOI : 10.1021/acs.jpcc.0c11589**

* A134; "CrI3 revisited with a many-body ab initio theoretical approach"
(第一原理多体手法によるヨウ化クロムの層間相互作用評価)

T. Ichibha, A. L. Dzubak, J. T. Krogel, V. R. Cooper, and F. A. Reboredo,
**Phys. Rev. Materials.** 5, 064006 (2021) [Q1-journal]
**DOI : 10.1103/PhysRevMaterials.5.064006**

* A133; "Exploring diamondlike lattice thermal conductivity crystals via feature-based transfer learning"
(転移学習による高熱伝導率化合物の探索)

S. Ju, R. Yoshida, C. Liu, S. Wu, K. Hongo, T. Tadano, J. Shiomi,
**Phys. Rev. Materials.** 5, 053801(2021) [Q1-journal]
**DOI : 10.1103/PhysRevMaterials.5.053801**

* A132; "Surface Study of Cu2SnS3 Using First‐Principles Density Functional Theory"
(第一原理計算を用いた太陽電池物質の表面解析)

R. Dahule, A. Raghav, A. T. Hanindriyo, K. Hongo, R. Maezono, E. Paanda,
**Adv. Theory Simul.** 2000315, 1-9(2021) [Q1-journal]
**DOI : 10.1002/adts.202000315**

* A131; "A Quantum Annealing Approach to Ionic Diffusion in Solids"
(量子アニーリングを用いた固体中イオン拡散の取扱い)

K. Utimula, T. Ichibha, G. I. Prayogo, K. Hongo, K. Nakano, R. Maezono,
**Sci. Rep.** 11, 7261 (2021) [Q1-journal]
**DOI : 10.1038/s41598-021-86274-3**

* A130; "Insights into the mechanical and electrical properties of metal-phosphorene interface: An ab-initio study with a wide range of metals"
(黒鱗半導体の電極に関する第一原理計算)

A. Ghaffar, M. D. Ganeriwala, K. Hongo, R. Maezono, N. R. Mohapatra,
**ACS Omega.** 6, 7795–7803 (2021) [Q1-journal]
**DOI : 10.1021/acsomega.0c06255**

* A129; "Intrinsic carbon-doping induced synthesis of oxygen vacancies-mediated TiO2 nanocrystals: Enhanced photocatalytic NO removal performance and mechanism"
(炭素ドーピングで誘起される酸素欠陥媒介チタン酸化物ナノ結晶の合成)

Z. Gu, Z. Cui, Z. Wang, K. S. Qin, Y. Asakura, T. Hasegawa, K. Hongo, R. Maezono, S. Yin,
**J. Catal.** 393, 179-189(2021) [Q1-journal]
**DOI : 10.1016/j.jcat.2020.11.025**

* A128; "Atomic forces by quantum Monte Carlo: application to phonon dispersion calculation"
(量子モンテカルロ法による力の計算: フォノン分散計算への応用)

K. Nakano, T. Morresi, M. Casula, R. Maezono, S. Sorella,
**Phys. Rev. B.** 103, L121110(2021) (2021) [Q1-journal]
https://doi.org/10.1103/PhysRevB.103.L121110

* A127; "Exploring Heat-Shielding Nanoparticle-Based Materials Via First-Principles Calculations and Transfer Learning",
(転移学習を用いた熱遮材料の探索)

T. Yoshida, R. Maezono, and K. Hongo,

**ACS Applied Nano Materials.** 4, 1932-1939(2021) [Q1-journal]
https://doi.org/10.1021/acsanm.0c03298

* A126; "Stochastic estimations of a total number of classes for the clusterings with too enormous samples to be accommodate into a clustering
engine,
(膨大なサンプルをクラスタリングするための, 確率的なクラスタ数推定方法)

K. Utimula, K. Nakano, G. I. Prayogo, K. Hongo, and R. Maezono,
**Adv. Theor. Sim.** 202000301 (2021) [Q1-journal]
https://doi.org/10.1002/adts.202000301

* A125; "Pressure-Induced CollapseTransitionin $BaTi_2Pn_2O$(Pn=As,Sb)with an Unusual Pn－Pn Bond Elongation",
(BaTi2Pn2O (Pn = As, Sb)における圧力によって誘起される特異な Pn-Pn の伸長を伴う構造相転移)

T. Yamamoto, T. Yajima, Z. Li, T. Kawakami, K. Nakano, T. Tohyama, T. Yagi, Y. Kobayashi, and H. Kageyama.
**Inorg. Chem.** 60, 2228-2233(2021) [Q1-journal]
https://doi.org/10.1021/acs.inorgchem.0c02989

* A124; "GaN bandgap bias caused by semi-core treatment in pseudopotentials analyzed by the diffusion Monte Carlo method",
(DMC によって明らかになった、擬ポテンシャルにおけるセミコア法に起因する GaN バンドギャップのバイアス)

Y. Nikaido, T. Ichibha, K. Nakano, K. Hongo, R. Maezono,
**AIP Adv.** 11 025225(2021) [Q2-journal]
https://doi.org/10.1063/5.0035047

* A123; "Synthesis, Electronic Structure, and Physical Properties of Layered Oxypnictides $Sr_2ScCrAsO_3$ and $Ba_3Sc_2Cr_2As_2O_5$",
(層状ニクタイド化合物の合成と電子構造)

S. P. K. Naik, Y. Iwasa, K. Kuramochi, Y. Ichihara, K. Kishio, K. Hongo, R. Maezono, T. Nishio, and H. Ogino,
**Inorg. Chem.** 60, 1930-1936 (2020) [Q1-journal]
https://dx.doi.org/10.1021/acs.inorgchem.0c03404

* A122; "Intrinsic electronic defect states of anatase using density functional theory",
(密度汎関数法によるアナターゼの欠陥準位解析)

A. Raghav, A.T. Hanindriyo, K. Utimula, M. Abbasnejad, R. Maezono, and E. Panda,
**Comp. Mat. Sci.** 184, 109925 (2020) [Q1-journal]
https://doi.org/10.1016/j.commatsci.2020.109925

* A121; "Carbon vacancies and hydroxyls in graphitic carbon nitride: Promoted photocatalytic NO removal activity and mechanism",

(カーボンナイトライド光触媒における炭素欠陥とヒドロキシル基)

Z. Gu, Z. Cui, Z. Wang, K. S. Qin, Y. Asakura, T. Hasegawa, S. Tsukuda, K. Hongo, R. Maezono, S. Yin,
**Appl. Catal. B.** 279. 119376 (2020) [Q1-journal]
https://doi.org/10.1016/j.apcatb.2020.119376

* A120; "General correlated geminal ansatz for electronic structure calculations: exploiting Pfaffians in place of determinant",
(電子状態計算における一般化されたジェミナル波動関数-パフィアン-の実装)

C. Genovese, T. Shirakawa, K. Nakano, S. Sorella,
**J. Chem. Theory Comput.** 16, 6114–6131 (2020) [Q1-journal]
https://doi.org/10.1021/acs.jctc.0c00165

* A119; "Hydride-reduced $Eu_2SrFe_2O_6$: a T-to-T′conversion enabling $Fe^{2}$+ in square planar coordination",
(水素化物によって還元された Eu2SrFe2O6: T -> T'変換により実現された Fe2+の平面 4 配位構造)

S.A. López-Paz, K. Nakano, J. Sanchez- Marcos, C. Tassel, M.A. Alario-Franco, H. Kageyama
**Inorganic Chemistry** 59, 12913-12919 (2020) [Q1-journal]
https://pubs.acs.org/doi/10.1021/acs.inorgchem.0c01982

* A118; "Octahedral morphology of NiO with (111) facet synthesized from the transformation of NiOHCl for $NO_x$ detection and degradation: Experiment and DFT calculation",
(NiO 表面のファセット成長に関する研究)

A. Hermawan, A.T. Hanindriyo, E.R. Ramadhan, Y. Asakura, T. Hasegawa, K. Hongo, M. Inada, R. Maezono, and S. Yin
**Inorg. Chem. Front.** 7, 3431-3442 (2020) [Q1-journal]
https://doi.org/10.1039/D0QI00682C

* A117; "Ab initio evaluation of complexation energies for cyclodextrin-drug inclusion complexes",
(シクロデキストリン-薬剤包接体の第一原理結合エネルギー評価)

K. Ogmhula, K. Hongo, R. Maezono, T. Ichibha,
**ACS Omega.** 5, 19371-19376 (2020) [Q1-journal]
https://doi.org/10.1021/acsomega.0c01059

* A116; "New layered perovskite family built from $[CeTa_2O_7]^-$ layers: coloring mechanism from unique multi-transitions",
(CeTa2O7 から合成した層状ペロブスカイトの着色メカニズム)

T.Hasegawa, A.Shigee, Y.Nishiwaki, M.Nagasako, A.T.Hanindriyo, K.Hongo, R.Maezono, T.Ueda, S.Yin,
**Chem.Commun.** 56, 8591-8594 (2020) [Q1-journal]
DOI/https://doi.org/10.1039/D0CC03466E

* A115; "Boron phosphide as a p -type transparent conductor: Optical absorption and transport through electron-phonon coupling",

(p 型透明伝導体リン化ボロンの光学特性と伝導性におけるフォノン効果)

V. Ha, B. Karasulu, R. Maezono, G. Brunin, J. B. Varley, G. Rignanese, B. Monserrat, G. Hautier,
**Phys. Rev. Mater.** 4, 65401 (2020) [Q1-journal]
DOI : 10.1103/PhysRevMaterials.4.065401

* A114; "Light Absorption Properties and Electronic Band Structures of Lead‐Vanadium Oxyhalide Apatites $Pb_5(VO_4)_3X$ (X=F, Cl, Br, I)",
(可視光による光触媒を目指した酸ハロゲン化アパタイトの合成と触媒能評価)

M. Nakamura, K. Oqmhula, K. Utimula, M. Eguchi, K. Oka, K. Hongo, R. Maezono, K. Maeda
**Chem Asian J.** 15, 540-545 (2020) [Q1-journal]
https://doi.org/10.1002/asia.201901692

* A113; "Synergy of Binary Substitution for Improving Cycle Performance in LiNiO2 Revealed by ab Initio Materials Informatics",
(リチウムイオン電池のサイクル特性向上に関するマテリアルインフォマティクス)

T. Yoshida, R. Maezono, K. Hongo
**ACS Omega.** 5, 13403-13408 (2020) [Q1-journal]
https://pubs.acs.org/doi/abs/10.1021/acsomega.0c01649

A112; "Machine-learning clustering technique applied to powder X-ray diffraction patterns to distinguish compositions of ThMn12-type alloys",
(機械学習を用いた ThM12 型合金の XRD 回折ピークパターン解析)

K. Utimula, R. Hunkao, M. Yano, H. Kimoto, K. Hongo, S. Kawaguchi, S. Suwanna, R. Maezono
**Adv. Theory Simul.** 3, 2000039 (2020) [Q1-journal]
https://doi.org/10.1002/adts.202000039

* A111; "Electrochemical Properties and Crystal Structure of $Li^+$ / $H^+$ Cation-Exchanged $LiNiO_2$",
($Li^+$/$H^+$カチオン交換された LiNiO2 の電気化学的性質と結晶構造)

T. Toma, R. Maezono, K. Hongo,
**ACS Appl. Energy Mater.** 3, 4078-4087 (2020) [Q1-journal]
https://doi.org/10.1021/acsaem.0c00602

* A110; "Ab initio thermodynamic properties of certain compounds in Nd-Fe-B system",
(Nd-Fe-B 磁石合金の計算熱力学第一原理アセスメント)

A.T. Hanindriyo, S. Sridar, K.C. Hari Kumar, K. Hongo, R. Maezono,
**Comp. Mater. Sci.** 180, 109696 (2020) [Q1-journal]
https://doi.org/10.1016/j.commatsci.2020.109696

* A109; " Two-Dimensional Perovskite Oxynitride $K_2LaTa_2O_6N$ with an $H^+/K^+$ Exchangeability in Aqueous Solution to Form Stable Photocatalyst
for Visible-Light $H_2$ Evolution",
(水素発生反応にかかる可視光光触媒水素の合成)

T. Oshima, T. Ichibha, K. Oqmhula, K. Hibino, S. Yamashita, K. Fuji, Y. Miseki, K. Hongo, D. Lu, R. Maezono, K. Sayama, M. Yashima, K. Kimoto, H. Kato, M. Kakihana, H. Kageyama, K. Maeda,
**Angew. Chem. Int. Ed.** 132, 2-10 (2020) [Q1-journal]
https://doi.org/10.1002/ange.202002534

* A108; "TurboRVB: a many-body toolkit for ab initio electronic simulations by quantum Monte Carlo",
(TurboRVB:第一原理量子モンテカルロ法による電子状態計算ツール)

K. Nakano, C. Attaccalite, M. Barborini, L. Capriotti, M. Casula, E. Coccia, M. Dagrada, C. Genovese, Y. Luo, G. Mazzola, A. Zen, S. Sorella,
**J. Chem. Phys.** 152, 204121 (2020) [Q1-journal]
https://doi.org/10.1063/5.0005037

* A107; "Speeding up the ab initio diffusion Monte Carlo by a smart lattice regularization",
(格子離散化による拡散量子モンテカルロ法の加速)

K. Nakano, R. Maezono, and S. Sorella,
**Phys. Rev. B.** 101, 155106 (2020) [Q1-journal]
https://doi.org/10.1103/PhysRevB.101.155106

* A106; "$\beta$ -sheet elasticity of peptide self-assembly mimic, PSAM, with a graftedsequence characterized by comprehensive analyses ofisomorphous crystals",
(同形結晶に対する包括的分析より明らかになった、接合されたシークエンスを持つ模擬自己集合性ペプチド(PSAM)の$\beta$シート弾性)

H. Fujiwara, K. Hongo, Y. Hori, N. Yoshida, K. Makabe,
**J. Mol. Liq.** 290, 15 (2019) [Q1-journal]
https://doi.org/10.1016/j.molliq.2019.111161

* A105; "Machine-learning-assisted discovery of polymers with high thermal conductivity using a molecular design algorithm",
(分子設計アルゴリズムを利用した、高熱伝導率をもつポリマーの機械学習による発見)

S. Wu, Y. Kondo, M. Kakimoto, B. Yang, H. Yamada, I. Kuwajima, G. Lambard, K. Hongo, Y. Xu, J. Shiomi, C. Schick, J. Morikawa, and R. Yoshida
**npj Computational Materials.** 5, 66, 111161 (2019) [Q1-journal]
https://doi.org/10.1038/s41524-019-0203-2

* A104; "Ti interstitial flows giving rutile $TiO_2$ reoxidation process enhanced in (001) surface",
(チタン酸化物表面再酸化の異方性に対する理論的解明)

T. Ichibha, A. Benali, K. Hongo, and R. Maezono
**Phys. Rev. Mater.** 3, 125801 (2019) [Q1-journal]
DOI: 10.1103/PhysRevMaterials.3.125801

* A103; "3D structured Laser engraves decorated with gold nanoparticle SERS chips for herbicide detection in environments",
(除草剤汚染を検知する 3 次元マイクロ流体表面増強ラマン散乱センサー)

R. Botta, P. Eiamchai, M. Horprathum, S. Limwichean, C. Chananonnawathorn, V. Patthanasettakul,
R. Maezono, A. Jomphoak and N. Nuntawong,
**Sensors and Actuators B: Chemical.** 304, **127327** (2020) [Q1-journal]
https://doi.org/10.1016/j.snb.2019.127327

* A102; "Chemical and structural stability of superconducting $In_5Bi_3$ driven by relativistic spin-orbit coupling",
(スピン軌道相互作用で安定化される超伝導体の結晶構造)

S. Chen, R. Maezono, J. Chen, F.M. Grosche, C.J. Pickard, and B. Monserrat.
**J. Phys. Mater.** 3, 015007 (2020) [Q1-journal]
https://iopscience.iop.org/article/10.1088/2515-7639/ab4c2b

* A101; "Inconsistencies in ab initio evaluations of non-additive contributions of DNA stacking energies"
(DNA スタッキングエネルギーの非加算性評価における、第一原理計算手法間での不一致性)

K.S. Qin, T. Ichibha, K. Hongo, and R. Maezono,
**Chem. Phys.** 529, 110554 (2020) [Q2-journal]
https://doi.org/10.1016/j.chemphys.2019.110554
arxiv:1807.04168

* A100; "A DFT+U Study of $H_2O$ Molecule Adsorption and Dissociation on Stoichiometric and Non-Stoichiometric CuO(111) Surface",
(酸化銅表面への水分子吸着に関する計算科学的研究)

F. Ahmad, M. Agusta, R. Maezono, H. Dipojono,
**J. Phys.: Condens. Matter.** 32, **045001 (2020)** [Q1-journal]
https://doi.org/10.1088/1361-648X/ab4b34

* A99; "Method for the Calculation of the Hamaker constants of Organic Materials by the Lifshitz Macroscopic Approach With DFT"
(有機材料の濡れ性に関する計算科学的研究)

H. Takagishi, T. Masuda, T. Shimoda, R. Maezono, and K. Hongo,
**J. Phys. Chem. A** 123, 8726-8733 (2019) [Q2-journal]

https://arxiv.org/abs/1906.08011
DOI/doi: 10.1021/acs.jpca.9b06433

* A98; "*Ab initio* search of polymer crystals with high thermal conductivity",
(高い熱伝導率を有するポリマーの計算科学的探索)

K. Utimula, T. Ichibha, R. Maezono, K. Hongo,
**Chem. Mater.** 13, 4649-4656 (2019) [Q1-journal]
DOI:10.1021/acs.chemmater.9b00020
arXiv:1811.06807

* A97; "All–electron quantum Monte Carlo with Jastrow single determinant Ansatz: application to the sodium dimer",
(全電子計算による量子モンテカルロ法電子状態計算法)

K. Nakano, R. Maezono, and S. Sorella,
**J. Chem. Theory Comput.** 15, 4044-4055 (2019) [Q1-journal]
https://arxiv.org/abs/1903.10731
https://doi.org/10.1021/acs.jctc.9b00295

* A96; "Synthesis, optical properties, and band structures of a series of layered mixed-anion compounds",
(複合アニオン物質における合成、光学特性、バンド構造の系統性)

Y. Iwasa, H. Ogino, D. Song, V.C. Agulto, K. Yamanoi, T. Shimizu, J. Ueda, K. Hongo, R. Maezono, S. Tanabe, and N. Sarukura.
**J. Mater. Sci.: Materials in Electronics** 30, 16827-16832 (2019) [Q2-journal]
DOI 10.1007/s10854-019-01380-3

* A95; "First-Principles Study of Structural Transition in $LiNiO_2$ and High Throughput Screening for Long Life Battery",
(リチウムイオン電池材料の長寿命化を目的とした計算科学的材料探索)

T. Yoshida, K. Hongo, and R. Maezono,
**J. Phys. Chem. C** 123, 14126-14131 (2019) [Q1-journal]
arXiv:1901.02261

* A94; "Density functional study of methyl butanoate adsorption and its C-O bonds cleavage on $MoS_2$-based catalyst with various Ni loads promoters",
(ニッケル被覆下での硫化モリブデン系触媒の分子吸着)

W.A.E. Prabowo, Subagjo, Nugraha, M.K. Agusta, A.G. Saputro, S. Rustad, R. Maezono, W.A. Dino, H.K. Dipojono,
**J. Phys. Condens. Matter** 31, 365001 (2019) [Q1-journal]
https://dx.doi.org/10.1088/1361-648X/ab2400

* A93; "Synthesis of $(Ba_{1-X}Sr_X)YSiO_5N$ and Discussion based on Structure Analysis and DFT Calculation",

($(Ba_{1-X}Sr_X)YSiO_5N$ のキャラクタリゼーションとフォトルミネッセンス)

T. Yasunaga, K. Hongo, K. Fujii, S. Yamamoto, R. Maezono, M. Yashima, M. Mitsuishi, H. Kato, M. Kobayashi, and M. Kakihana,
**J. Sold State Chem**. 276, 266-271 (2019) [Q2-journal]
**DOI: 10.1016/j.jssc.2019.05.012**

* A92; "First-principles anharmonic vibrational study of the structure of calcium silicate under lower mantle conditions",
(下部マントル条件でのケイ酸カルシウムの非調和格子振動)

J.C.A. Prentice, R. Maezono, and R.J. Needs,
**Phys. Rev. B** 99, 064101 (2019) [Q1-journal]
DOI: 10.1103/PhysRevB.99.064101

* A91; "A new ab initio modeling scheme for the ion self-diffusion coefficient applied to the ε-$Cu_3Sn$ phase of the Cu–Sn alloy",
(無鉛ハンダ物質中のイオン移動に対する新しいモデリング)

T. Ichibha, G.I. Prayogo, K. Hongo, R. Maezono,
**Phys. Chem. Chem. Phys**. 21, 5158-5164 [Q1-journal]
DOI: 10.1039/C8CP06271D

* A90; "Crystal structure analysis and evidence of mixed anion coordination at the $Ce^{3+}$ site in $Y_3Al_2(Al,Si)_3(O,N)_{12}$ oxynitride garnet phosphor",
(高圧合成による酸化物ガーネット蛍光体の作製と光学特性)

K. Asami, M. Shiraiwa, J. Ueda, K. Fujii, K. Hongo, R. Maezono, M. Brik, M. Yashima, S. Tanabe,
**J. Mater. Chem. C** 7, 1330-1336 (2019) [Q1-journal]
DOI: 10.1039/C8TC04980G

* A89; "High pressure synthesis of $A_2NiO_2Ag_2Se_2$ (A = Sr, Ba) with a high spin $Ni^{2+}$ in square planar coordination",
(平面四配位場におけるニッケルイオンの高スピン状態)

Y. Matsumoto, T. Yamamoto, K. Nakano, H. Takatsu, T. Murakami, K. Hongo, R. Maezono, H. Ogino, D. Song, C.M. Brown, C. Tassel, H. Kageyama,
**Angew. Chem. Int. Ed.** 58, 756-759 (2019) [Q1-journal]

* A88; "Assessing the performance of the Tran-Blaha modified Becke-Jonhson exchange potential for optical constants of semiconductors sin the UV-Vis light region",
(Tran-Blaha 汎関数の半導体の紫外-可視光域の光学定数に対する予測性能の検証)

K. Nakano, and T. Sakai
**J. Appl. Phys.** 123, 015104 (2018) [Q1-journal]
DOI:10.1063/1.5006170

* A87; "Estimation of maximum absorption wavelength of polymethine dyes in visible and near-infrared region based on time-dependent density functional theory",
(TD-DFT 計算に基づいたポリメチン色素化合物の可視-近赤外域の最大吸収波長の予測)

K. Nakano, T. Konishi, and Y. Imamura,
**Chem. Phys.** 518, 15-24 (2019) [Q1-journal]
DOI/10.1016/j.chemphys.2018.11.002
arXiv 1911.08071 (2019)

* A86; "Light Absorption Properties and Electronic Band Structures of Lead Titanium Oxyfluoride Photocatalysts $Pb_2Ti_4O_9F_2$ and $Pb_2Ti_2O_{5.4}F_{1.2}$",
(鉛チタン酸フッ化物光触媒のバンドエンジニアリング)

H. Wakayama, K. Utimura, T. Ichibha, R Kuriki, K. Hongo, R. Maezono, K. Oka, and K. Maeda,
**J. Phys. Chem. C** 122, 26506–26511 (2018) [Q1-journal]
DOI: 10.1021/acs.jpcc.8b08953

* A85; "Bandgap reduction of photocatalytic $TiO_2$ nanotube by Cu doping",
(Cu ドープした $TiO_2$ ナノチューブの光触媒特性)

S.K. Gharaei, M. Abbasnejad, R. Maezono,
**Sci. Rep.** 8, 14192 (2018) [Q1-journal]
DOI:10.1038/s41598-018-32130-w

* A84; "Quantum Monte Carlo calculations of energy gaps from first principles"
(第一原理量子モンテカルロ法によるエネルギーギャップ計算)

R.J. Hunt, M. Szyniszewski, G.I. Prayogo, R. Maezono, N.D. Drummond,
**Phys. Rev. B** 98, 075122 (2018) [Q1-journal]
DOI: 10.1103/PhysRevB.98.075122

* A83; "Development of persistent phosphor of $Eu^{2+}$ doped $Ba_2SiO_4$ by $Er^{3+}$ co-doping based on vacuum referred binding energy diagram",
($Eu^{2+}$と $Er^{3+}$の共ドープによる長残光蛍光体の開発)

K. Asami, J. Ueda, K. Yasuda, K. Hongo, R. Maezono, M.G. Brik, S. Tanabe,
**Opt. Mater**. 84, 436-441 (2018) [Q1-journal]
https://doi.org/10.1016/j.optmat.2018.07.021

* A82; "Host-Guest Interactions of Plumbagin with β-Cyclodextrin, Dimethyl-β-Cyclodextrin and Hydroxypropyl-β-Cyclodextrin: Semi-Empirical
Quantum Mechanical PM6 and PM7 Methods"

(半経験的手法によるシクロデキストリンのホストゲスト相互作用解析)

O. Srihakulung, R. Maezono, P. Toochinda, W. Kongprawechnon, A. Intarapanich, L. Lawtrakul,
**Sci. Pharm.** 86, 20:1-11 (2018) [Q2-journal]
https://doi.org/10.3390/scipharm86020020

* A81; "A Stable, Narrow-Gap Oxyfluoride Photocatalyst for Visible-Light Hydrogen Evolution and Carbon Dioxide Reduction",
(可視光二酸化炭素還元を用途とした酸フッ化物光触媒)

R. Kuriki, T. Ichibha, K. Hongo, D. Lu, R Maezono, H. Kageyama, O. Ishitani, K. Oka, and K. Maeda,
**J. Am. Chem. Soc**. 140, 6648-6655 (2018) [Q1-journal]
DOI: 10.1021/jacs.8b02822

* A80; "Undoped Layered Perovskite Oxynitride $Li_2LaTa_2O_6N$ for Photocatalytic $CO_2$ Reduction with Visible-Light",
(可視光による二酸化炭素還元を目的としたペロブスカイト型酸窒化物の合成と触媒能評価)

T. Oshima, T. Ichibha, K.S. Qin, K. Muraoka, J.J.M. Vequizo, K. Hibino, R. Kuriki, S. Yamashita, K. Hongo, T. Uchiyama, K. Fujii, D. Lu, R. Maezono, A. Yamakata, H Kato, K. Kimoto, M. Yashima, Y. Uchimoto, M. Kakihana, O. Ishitani, H. Kageyama and K. Maeda,
**Angew. Chem. Int. Ed.** 57, 8154-8158 (2018) [Q1-journal]
doi: 10.1002/anie.201803931

* A79; " Stabilization Mechanism of the Tetragonal Structure in a Hydrothermally Synthesized BaTiO3 Nanocrystal",
(水熱合成された BaTiO3 のナノ結晶における正方晶構造の安定メカニズム)

K. Hongo, S. Kurata, A. Jomphoak, M. Inada, K. Hayashi, R. Maezono,
**Inorg. Chem.** 57, 5413-5419 (2018) [Q1-journal]
DOI: 10.1021/acs.inorgchem.8b00381

* A78; " Hypervalent Bismuthides La3MBi5 (M = Ti, Zr, Hf) and Related Antimonides: Absence of Superconductivity ",
(超原子価ビスマス化合物における超伝導相の不在)

T. Murakami, T. Yamamoto, F. Takeiri, K. Nakano, and H. Kageyama,
**Inorg. Chem.** 56, 5041-5045 (2017) [Q1-journal]
DOI: 10.1021/acs.inorgchem.7b00031

* A77; "Adhesion of Electrodes on Diamond (111) Surface: A DFT Study",
(ダイアモンド半導体電極の耐剥離性と伝導性)

T. Ichibha, K. Hongo, I. Motochi, N.W. Makau, G.O. Amolo, R. Maezono,
**Diam. Relat. Mater.** 81, 168–175 (2018) [Q2-journal]
https://doi.org/10.1016/j.diamond.2017.12.008

* A76; "Density Functional Theory Simulations of Aluminium Alkoxide and Fluoride",

(アルミアルコキシドとフッ化物の電子状態計算)

A. Jomphoak, T. Onjun, K. Hongo, R. Maezono,
**Int. J. New Tech. Res.** (IJNTR) 3, 12-14 (2017)

* A75; " Valence Band Engineering of Layered Bismuth Oxyhalides toward Stable Visible-Light Water Splitting: Madelung Site Potential Analysis",

(安定な可視光水分解を実現するための、マーデルングポテンシャル分析を利用した、層状ビスマスオキシハライドの価電子バンド構造制御)

D. Kato, K. Hongo, R. Maezono, M. Higashi, H. Kunioku, M. Yabuuchi, H. Suzuki, Z. Chengchao, K. Nakano, R. Abe, and H. Kageyama,
**J. Am. Chem. Soc.** 139, 18725–18731 (2017) [Q1-journal]
DOI: 10.1021/jacs.7b11497

* A74; "Investigation into structural phase transitions in layered titanium-oxypnictides by a computational phonon analysis"

(第一原理フォノン計算による、層状チタンニクタイド酸化物の構造相転移に関する研究)

K. Nakano, K. Hongo, and R. Maezono,
**Inorg. Chem.** 56, 13732–13740 (2017) [Q1-journal]
DOI: 10.1021/acs.inorgchem.7b01709

* A73; " A computational scheme to evaluate Hamaker constants of molecules with practical size and anisotropy",

(量子モンテカルロ法による濡れ性の研究)

K. Hongo and R. Maezono,
**J. Chem. Theory Comput.** 13, 5217-5230 (2017) [Q1-journal]
DOI: 10.1021/acs.jctc.6b01159

* A72; "Diffusion quantum Monte Carlo study of excitonic complexes in two-dimensional transition-metal dichalcogenides",

(層状遷移金属ダイカルゴゲナイトにおける励起子複合体のモット・ワニエ・ケルディッシュモデル)

E. Mostaani, M. Szyniszewski, C.H. Price, R. Maezono, M. Danovich, N.D. Drummond, and V.I. Fal'ko,
**Phys. Rev. B** 96, 75431 (2017) [Q1-journal]
DOO: 10.1103/PhysRevB.96.075431

* A71; "Influence of endohedral confinement of atoms on structural and dynamical properties of the C60 fullerene",

(C60 フラーレンの内包原子に関する第一原理計算)

A.J. Etindele, R. Maezono, R.L.M. Melono, and O. Motapon
**Chem. Phys. Lett.** 685C, 395-400 (2017) [Q2-journal]
https://doi.org/10.1016/j.cplett.2017.07.074

* A70; "New Insight into the Ground State of FePc: A Diffusion Monte Carlo Study"
(鉄フタロシアニンの配位子場モデルに対する考察)

T. Ichibha, Z. Hou, K. Hongo, and R. Maezono,
**Sci. Rep.** 7, 2011 (2017) [Q1-journal]
DOI:10.1038/s41598-017-01668-6

* A69; "Computational design of Ni-Zn based catalyst for direct hydrazine fuel cell catalyst using density functional theory"
(ヒドラジン燃料電池用途触媒の計算科学的デザイン)

A.T. Hanindriyo, TB.M.Y.Y. Prawiraa, M.K. Agusta, R. Maezono, H.K. Dipojono.
**Procedia Eng**. 170, 148-153 (2017)
doi:10.1016/j.proeng.2017.03.034

* A68; "Quantum Monte Carlo study of the energetics of rutile, anatase, brookite and columbite $TiO_2$ polymorphs"
(チタン酸化物多形の量子モンテカルロ法電子状態計算と非調和格子振動)

J. Trail, B. Monserrat, P.L. Rios, R. Maezono, and R.J. Needs,
**Phys. Rev. B** 95, 121108(R) (2017) [Q1-journal]
DOI: 10.1103/PhysRevB.95.121108

* A67; "Bayesian Molecular Design with A Chemical Language Model"
(ベイズ推定を用いた分子構造探査)

H. Ikebata, K. Hongo, T. Isomura, R. Maezono, and R.Yoshida,
**J. Comput. Aided Mol. Des.** 31, 379-391 (2017) [Q2-journal]
DOI 10.1007/s10822-016-0008-z

* A66; "Selectivity of CO and NO adsorption on ZnO (0002) surfaces: A DFT investigation"
(ZnO 表面における CO 分子/NO 分子の選択的吸収)

Nugraha, A.G. Saputro, M.K. Agusta, B. Yuliarto, H.K. Dipojono, F. Rusydi, and R. Maezono,
**Appl. Surf. Sci.** 410, 373–382 (2017) [Q1-journal]
http://dx.doi.org/10.1016/j.apsusc.2017.03.009

* A65; "Density functional theory of graphene/Cu phthalocyanine composite material"
(グラフェン上の銅フタロシアニン分子に関する第一原理計算)

A. Jomphoak, R. Maezono, T. Onjun,
**Surf. Coat Tech.** 306, 236–239 (2016) [Q1-journal]
DOI: 10.1016/j.surfcoat.2016.06.015

* A64; "First-Principles Molecular Dynamics Study on Helium-filled Carbon Nanotube"
(カーボンナノチューブ中のヘリウムに関する第一原理分子動力学計算)

M.K. Agusta, I. Prasetiyo, A.G. Saputro, R. Maezono, H.K. Dipojono
**J. Phys. Conf. Ser.** 739, 12081 (2016)
DOI:10.1088/1742-6596/739/1/012081

* A63; "Density functional study of adsorptions of $CO_2$, $NO_2$ and $SO_2$ molecules on Zn(0002) surfaces"
(亜鉛表面上への二酸化炭素、二酸化窒素、二酸化硫黄分子の吸着)

Nugraha, A.G. Saputro, M.K. Agusta, B. Yuliarto, H.K. Dipojono, R. Maezono
**J. Phys. Conf. Ser.** 739 (2016), 12080 (2016) [Q4-journal]
DOI:10.1088/1742-6596/739/1/012080

* A62; "DFT study of the formation on Ni(111) surface doped by transition metals [Ni(111)-M; M=Cu, Pd, Pt, Rh]"
(ニッケル表面にドープされた遷移金属元素の生成エネルギー評価)

Nugraha, A.G. Saputro, M.K. Agusta, F. Rusydi, R. Maezono, H.K. Dipojono,
**J. Phys. Conf. Ser.** 739 (2016), 12082 (2016)
DOI:10.1088/1742-6596/739/1/012082

* A61; "Phonon dispersions and Fermi surfaces nesting explaining the variety of charge ordering in titanium-oxypnictides superconductors"
(層状チタンニクタイド酸化物の電荷整列多様性の根源となるフォノン分散とネスティング)

K. Nakano, K. Hongo, and R. Maezono,
**Sci. Rep.** 6, 29661 (2016) [Q1-journal]
doi:10.1038/srep29661

* A60; "Electrical Properties of Epitaxial Thin Films of Oxyhydrides ATiO3-xHx (A = Ba and Sr)"
(エピタキシャル成長させた酸水素化物薄膜の電気的性質)

G. Bouilly, T. Yajima, T. Terashima, W. Yoshimune, K. Nakano, C. Tassel, Y. Kususe, K. Fujita, K. Tanaka, T. Yamamoto, Y. Kobayashi, and H. Kageyama
**Chem. Mater.** 27, 6354-6359 [Q1-journal]
DOI: 10.1021/acs.chemmater.5b02374

* A59; "Emergence of a Kondo singlet state with the Kondo temperature well beyond 1,000K in the proton-embedded electron gas"
(原子埋め込み系における近藤シングレット状態の出現)

Y. Takada, R. Maezono, and K. Yoshizawa,
**Phys. Rev. B.** 92, 155140:1-11 (2015) [Q1-journal]
DOI:http://dx.doi.org/10.1103/PhysRevB.92.155140

* A58; "QMC and phonon study of super-hard cubic boron carbon nitride"
(立方晶窒化ボロンおよび炭素窒化ボロンの体積弾性率)

M.O. Atambo, N.W. Makau, G.O. Amolo, and R. Maezono,
**Mater. Res. Express** 2, 105902:1-7 (2015) [Q2-journal]
DOI: 10.1088/2053-1591/2/10/105902.

* A57; "Diffusion Monte Carlo study of Para-Diiodobenzene Polymorphism Revisited"
(DIB 分子結晶の量子拡散モンテカルロ法電子状態計算)

K. Hongo and T. Iitaka, M. Watson, A. Aspuru-Guzik, and R. Maezono,
**J. Chem. Theory Comput.**, 11, 907-917 (2015) [Q1-journal]
DOI: 10.1021/ct500401p

* A56; "Superconductivity in $LaPd_2As_2$ with a collapsed 122 structure"
(122 型の結晶構造を持つ LaPd2As2 における超伝導)

S. Ganesanpotti, T. Yajima, K. Nakano, Y. Nozaki, T. Yamamoto, C. Tassel, Y. Kobayashi, and H. Kageyama,
**J. Alloys Compd.**, 613, 370-374 (2014) [Q1-journal]
DOI: 10.1016/j.jallcom.2014.06.054

* A55; "Superconducting properties of $BaTi_2Pn_2O$ (Pn = Sb, Bi)"
(超伝導物性)

T. Yajima, K. Nakano, Y. Nozaki, and H. Kageyama
**Physica C Supercond** 504, 36-38 [Q2-journal]
DOI: 10.1016/j.physc.2014.02.018

* A54; "Anomalous non-additive dispersion interactions in systems of three one-dimensional wires"
(金属ナノワイヤ間の分散力相互作用と非加算性)

A.J. Misquitta, R. Maezono, N.D. Drummond, A.J. Stone, and R.J. Needs.,
**Phys. Rev. B** 89, 045140:1-9 (2014) [Q1-journal]
DOI: 10.1103/PhysRevB.89.045140

* A53; "LaPd2Sb2: A pnictide superconductor with CaBe2Ge2 type structure"
(CaBe2Ge2 型構造を持つ超伝導体:LaPd2Sb2)

S. Ganesanpotti, T. Yajima, T. Tohyama, Z. Li, K. Nakano, Y. Nozaki, C. Tassel, Y. Kobayashi, and H. Kageyama
**J. Alloys Compd.** 583, 151-154 [Q1-journal]
DOI: 10.1016/j.jallcom.2013.08.005

* A52; "Gold-standard coupled-cluster study of the ground-state chromium dimer cation"
(クロム二量体カチオンの結合クラスター計算)

Y. Yamad, K. Hongo, K. Egashira, Y. Kita, U. Nagashima M. Tachikawa,
**Chem. Phys. Lett.** 555, 84-86 (2013) [Q2-journal]
DOI: 10.1016/j.cplett.2012.11.017

* A51; "$T_c$ Enhancement by Aliovalent Anionic Substitution in Superconducting $BaTi_2(Sb_{1-x}Sn_x)_2O$"
($BaTi_2(Sb_{1-x}Sn_x)_2O$:異原子価置換による Tc の上昇)

K. Nakano, T. Yajima, F. Takeiri, M. A. Green, J. Hester, Y. Kobayashi, and H. Kageyama,
**J. Phys. Soc. Jpn.** 82, 74707 (2013) [Q2-journal]
DOI: 10.7566/JPSJ.82.074707

* A50; "Hierarchically porous monoliths based on N-doped reduced titanium oxides and their electric and electrochemical properties"
(窒素ドープされたチタン酸化物を利用した階層的多孔質モノリスの電気的, 及び電気化学的特性)

G. Hasegawa, T. Sato, K. Kanamori, K. Nakano, T. Yajima, Y. Kobayashi, H. Kageyama, T. Abe, and K. Nakanishi,
**Chem. Mater.** 25, 3504-3512 (2013) [Q1-journal]
DOI: 10.1021/cm401933a

* A49; "S-wave superconductivity in superconducting $BaTi_2Sb_2O$ revealed by $^{121/123}$Sb-NMR/nuclear quadrupole resonance measurements"
($^{121/123}$Sb-NMR によって明らかになった $BaTi_2Sb_2O$ における s 波超伝導)

S. Kitagawa, K. Ishida, K. Nakano, T. Yajima, and H. Kageyama,
**Phys. Rev. B.** 87, 60510 (2013) [Q1-journal]
DOI: 10.1103/PhysRevB.87.060510

* A48; "Muon spin relaxation and electron/neutron diffraction studies of BaTi2(As1-xSbx)2O: Absence of static magnetism and superlattice reflections"
(ミュオンスピン回転, 及び電子/中性子線回折によって判明した BaTi2(As1-xSbx)2O における静磁場と超格子の不在)

Y. Nozaki, K. Nakano, T. Yajima, H. Kageyama, B. Frandsen, L. Liu, S. Cheung, T. Goko, Y. J. Uemura, T. S. J. Munsie, T. Medina, G. M. Luke, J. Munevar, D. Nishio-Hamane, and C. M. Brown,
**Phys. Rev. B.** 88, 214506 (2013) [Q1-journal]
DOI: 10.1103/PhysRevB.88.214506

* A47; "Two Superconducting Phases in the Isovalent Solid Solutions $BaTi_2Pn_2O$ (Pn = As, Sb, and Bi)"
($BaTi_2Pn_2O$ の等原子価置換固溶体における 2 つの超伝導相)

T. Yajima, K. Nakano, F. Takeiri, Y. Nozaki, Y. Kobayashi, and H. Kageyama,
**J. Phys. Soc. Jpn.** 82, 033705 (2013) [Q2-journal]

DOI: 10.7566/JPSJ.82.033705

* A46; "Excitons and biexcitons in symmetric electron-hole bilayers"
(半導体二層膜の中密度域におけるバイエキシトン気体)

R. Maezono, Pablo Lopez Rios, T. Ogawa, and R.J. Needs,
**Phys. Rev. Lett.** 110, 216407:1-5 (2013) [Q1-journal]
DOI: 10.1103/Phys. Rev. Lett.110.216407

* A45; "The Importance of Electron Correlation on Stacking Interaction of Adenine-Thymine Base-Pair Step in B-DNA: A Quantum Monte Carlo Study"
(DNA の塩基間引力に対する量子モンテカルロ法電子状態計算)

K. Hongo N.T. Cuong, and R. Maezono.
**J. Chem. Theory Comput.** 9, 1081–1086 (2013) [Q1-journal]
DOI: 10.1021/ct301065f

* A44; "GPGPU for orbital function evaluation with a new updating scheme"
(GPGPU に適した量子モンテカルロ電子状態計算法における新しい配位更新法)

Y. Uejima and R. Maezono.
**J. Comput. Chem.** 34, 83-94 (2013) [Q1-journal]
DOI: 10.1002/jcc.23106

* A43; "A benchmark quantum monte carlo study of molecular crystal polymorphism: A challenging case for density-functional theory"
(量子モンテカルロ計算による分子結晶多形予測)

M. A. Watson, K. Hongo, T. Iitaka, A. Aspuru-Guzik,
**ACS Symp. Ser.** 1094, 101-117 (2012) [Q3-journal]
DOI: 10.1021/bk-2012-1094.ch009

* A42; "Synthesis and physical properties of the new oxybismuthides BaTi2Bi2O and (SrF)2Ti2Bi2O with a d1 square net"
(d1 正方格子を持つ新規ビスマス超伝導体:BaTi2Bi2O, (SrF)2Ti2Bi2O の合成と物性)

T. Yajima, K. Nakano, F. Takeiri, J. Hester, T. Yamamoto, Y. Kobayashi, N. Tsuji, J. Kim, A. Fujiwara, and H. Kageyama,
**J. Phys. Soc. Jpn.** 82, 013703 (2012) [Q2-journal]
DOI: 10.7566/JPSJ.82.013703

* A41; "Superconductivity in $BaTi_2Sb_2O$ with a $d^1$ square lattice."
($d^1$ 正方格子を持つ新規超伝導体:$BaTi_2Sb_2O$)

T. Yajima, K. Nakano, F. Takeiri, T. Ono, Y. Hosokoshi, Y. Matsushita, J. Hester, Y. Kobayashi, and H. Kageyama,

**J. Phys. Soc. Jpn.** 81, 103706 (2012) [Q2-journal]
DOI: 10.1143/JPSJ.81.103706

* A40; " Quantum Monte Carlo study of pressure-induced B 3－ B 1 phase transition in GaAs"
(化合物半導体の構造相転移に関する量子モンテカルロ法電子状態計算)

C.N.M. Ouma, M.Z. Mapelu, N.W. Makau, G.O. Amolo, and R. Maezono,
**Phys. Rev. B** 86 104115:1-7 (2012) [Q1-journal]
DOI: 10.1103/PhysRevB.86.104115

* A39; "Quantum Monte Carlo study of high-pressure cubic $TiO_2$"
(チタン酸化物の量子モンテカルロ法電子状態計算)

M. Abbasnejad, E. Shojaee, M.R. Mohammadizadeh, M. Alaei, and R. Maezono,
**Appl. Phys. Lett.** 100, 261902 (2012) [Q1-journal]
DOI: 10.1063/1.4730608

* A38; "Structural, electronic, and dynamical properties of Pca21-$TiO_2$ by first principles"
(チタン酸化物の密度汎関数計算)

M. Abbasnejad, M.R. Mohammadizadeh and R. Maezono,
**Europhys. Lett.** 97, 56003:1-6 (2012) [Q2-journal]
DOI: 10.1209/0295-5075/97/56003

* A37; "A Benchmark quantum Monte Carlo study of the ground state chromium dimer"
(クロム二量体の結合に関する第一原理量子モンテカルロ計算)

K. Hongo and R. Maezono,
**Int. J. Quant. Chem.** 112, 1243-1255 (2012) [Q2-journal]
DOI: 10.1002/qua.23113

* A36; "A quantum monte carlo study of the ground state chromium dimer"
(クロム二量体の結合に関する第一原理量子モンテカルロ計算)

K. Hongo and R. Maezono,
**ACS Symp. Ser.** 1094, 91-99(2012) [Q3-journal]
DOI: 10.1021/bk-2012-1094.ch008

* A35; "Ab initio quantum Monte Carlo study of the binding of a positron to alkali-metal hydrides"
(アルカリハライドによるポジトロン束縛の量子モンテカルロ法電子状態計算)

Y. Kita, R. Maezono, M. Tachikawa, M.D. Towler, and R.J. Needs,

**J. Chem. Phys.** 135, 54108:1-5 (2009) [Q1-journal]
https://doi.org/10.1063/1.3620151

* A34; "Quantum Monte Carlo simulations with RANLUX random number generator"
(量子モンテカルロ法電子状態計算における疑似乱数)

K. Hongo and R. Maezono,
**Progress in NUCLEAR SCIENCE and TECHNOLOGY**, Vol. 2, pp.51-55 (2011)

* A33; "Acceleration of a QM/MM-QMC simulation using GPU"
(GPU を用いた FMO-QMC 計算の高速化)

Y. Uejima, T. Terashima and R. Maezono,
**J. Comput. Chem.** 32, 2264-2272 (2011) [Q1-journal]
DOI: 10.1002/jcc.21809

* A32; "Failure of conventional density functionals for the prediction of molecular crystal polymorphism: A quantum monte carlo study"
(従来密度汎関数の分子結晶多形予測不全：量子モンテカルロ検証)

K. Hongo, M. A. Watson, R. S. Sánchez-Carrera, T. Iitaka, A. Aspuru-Guzik,
**J. Phys. Chem. Lett** 1, 1789-1794(2010) [Q1-journal]
DOI: 10.1021/jz100418p

* A31; "Unified interpretation of Hund's first and second rules for 2p and 3p atoms"
(フント第一・第二則の統一的解釈)

T. Oyamada, K. Hongo, Y. Kawazoe, H. Yasuhara,
**J. Chem. Phys.** 133, 164113(2010) [Q1-journal]
DOI: 10.1063/1.3488099

* A30; "Size dependence of the bulk modulus of semiconductors nanocrystals"
(半導体ナノ結晶における体積弾性率のサイズ依存性)

R. Cherian, C. Gerard, P. Mahadevan, N.T. Cuong and R. Maezono,
**Phys. Rev. B** 82, 235321:1-7 (2010) [Q1-journal]
DOI: 10.1103/PhysRevB.82.235321

* A29; "Optimum and efficient sampling for variational quantum Monte Carlo"
(量子モンテカルロ法における分布急尖性を考慮したサンプリング法)

J.R. Trail and R. Maezono,
**J. Chem. Phys.** 133, 174120 (2010) [Q1-journal]

DOI: 10.1063/1.3488651

* A28; "Diamond to beta-tin phase transition in Si within quantum Monte Carlo"
(珪素固体の構造相転移に関する量子モンテカルロ計算)

R. Maezono, N.D. Drummond, A. Ma, and R.J. Needs,
**Phys. Rev. B** 82, 184108 (2010) [Q1-journal]
DOI: 10.1103/PhysRevB.82.184108

* A27; "Random number generators tested on quantum Monte Carlo simulations"
(量子モンテカルロ法における乱数生成法)

K. Hongo, R. Maezono, K. Miura,
**J. Comput. Chem**. 31, 2186–2194 (2010) [Q1-journal]
DOI: 10.1002/jcc.21509

* A26; "Ab initio quantum Monte Carlo study of the positronic hydrogen cyanide molecule"
(HCN 分子へのポジトロン親和性に関する第一原理量子モンテカルロ計算)

Y. Kita, R. Maezono, M. Tachikawa, M.D. Towler, and R.J. Needs,
**J. Chem. Phys.**, 131, 134310:1-6 (2009) [Q1-journal]
DOI: 10.1063/1.3239502

* A25; "Optimization of Many-body Wave function"
(多体波動関数の最適化)

R. Maezono,
**J. Comput. Theor. Nanosci.**, 6, 2474-2482 (2009) [Q4-journal]
DOI: 10.1166/jctn.2009.1308

* A24; "Quantum Monte Carlo study of porphyrin transition metal complexes"
(第一原理量子モンテカルロ法によるポルフィリン分子の計算)

J. Koseki, R. Maezono, M. Tachikawa, M.D. Towler, and R.J. Needs,
**J. Chem. Phys.** 129, 085103:1-5 (2008) [Q1-journal]
DOI: 10.1063/1.2966003

* A23; "Ab initio interpretation of Hund's rule for the methylene molecule: Variational optimization of its molecular geometries and energy component analysis"
(メチレン分子のフント則の正しい解釈)

Y. Maruyama, K. Hongo, M. Tachikawa, Y. Kawazoe, H. Yasuhara,

**Int. J. Quant. Chem.** 108, 731-743(2008) [Q2-journal]
DOI: 10.1002/qua.21541

* A22; "Diffusion Monte Carlo study of correlation in the hydrogen molecule"
(拡散モンテカルロ法による水素分子の電子相関)

K. Hongo, Y. Kawazoe, H. Yasuhara,
**Int. J. Quant. Chem.** 107, 1459-1467(2007) [Q2-journal]
DOI: 10.1002/qua.21277

* A21; "Correct interpretation of hund's rule and chemical bonding based on the virial theorem"
(ビリアル定理に基づくフント則と化学結合の正しい解釈)

K. Hongo, T. Oyamada, Y. Maruyama, Y. Kawazoe, H. Yasuhara,
**Mater. Trans.** 48, 662-665(2007) [Q3-journal]
DOI: 10.2320/matertrans.48.662

* A20; "Correct interpretation of Hund's multiplicity rule for atoms and molecules"
(原子・分子のフント多重度則の正しい解釈)

K. Hongo, T. Oyamada, Y. Maruyama, Y. Kawazoe, H. Yasuhara,
**J. Magn. Magn. Mater.** 310, e560-e562(2007) [Q2-journal]
DOI: 10.1016/j.jmmm.2006.10.894

* A19; "Fragmentation method combined with Quantum Monte Carlo calculations"
(第一原理量子モンテカルロ法とフラグメント分子軌道法を組み合わせた生体分子の計算)

R. Maezono, H. Watanabe, S. Tanaka, M.D. Towler, and R.J. Needs,
**J. Phys. Soc. Jpn.** 76, 064301:1-5 (2007) [Q2-journal]
DOI: 10.1143/jpsj.76.064301

* A18; "Equation of state and Raman frequency of diamond from quantum Monte Carlo simulations"
(ダイアモンド固体の状態方程式とラマン振動数に関する第一原理量子モンテカルロ計算)

R. Maezono, A. Ma, M.D. Towler, and R.J. Needs,
**Phys. Rev. Lett.,** 98, 025701:1-4 (2007) [Q1-journal]
DOI: 10.1103/PhysRevLett.98.025701

* A17; "The influence of correlation on the interpretation of Hund's multiplicity rule: A quantum Monte Carlo study"
(量子モンテカルロ法によるフント多重度則の解釈)

T. Oyamada, K. Hongo, Y. Kawazoe, H. Yasuhara,

**J. Chem. Phys.** 125, 14101(2006) [Q1-journal]
DOI: 10.1063/1.2209692

* A16; "Diffusion Monte Carlo study of atomic systems from Li to Ne"
(軽原子系の拡散モンテカルロ計算)

K. Hongo, Y. Kawazoe, H. Yasuhara,
**Mater. Trans.** 47 2612-2616(2006) [Q3-journal]
DOI: 10.2320/matertrans.47.2612

* A15; " An orbital-dependent correlation energy functional in density-functional theory for the study of strongly-correlated electronic systems"
(密度汎関数理論における軌道依存相関エネルギー汎関数)

H. Yasuhara, M. Higuchi, S. Ishii, K. Hongo, Y. Kawazoe,
**Mater. Trans.** 45, 1402-1410 (2004) [Q3-journal]
DOI: 10.2320/matertrans.45.1402

* A14; "Interpretation of Hund's multiplicity rule for the carbon atom"
(炭素原子におけるフント則の解釈)

K. Hongo, R. Maezono, Y. Kawazoe, H. Yasuhara, M.D. Towler, and R.J. Needs,
**J. Chem. Phys.** 121, 7144-7147 (2004) [Q1-journal]
DOI: 10.1063/1.1795151

* A13; "Quantum Monte Carlo study of atomic and solid sodium"
(ナトリウム固体の量子モンテカルロ計算)

R. Maezono, M.D. Towler, Y. Lee and R.J. Needs,
**Phys. Rev. B** 68, 165103:1-9 (2003) [Q1-journal]
DOI :10.1103/PhysRevB.68.165103

* A12; "Jahn-Teller effect and Electron correlation in manganites"
(マンガン酸化物における電子相関とヤーンテラー効果)

R. Maezono and N. Nagaosa,
**Phys. Rev. B** 67, 064413 (2003) [Q1-journal]
DOI: 10.1103/PhysRevB.67.064413

* A11; " Multiscale simulation of cluster growth and deposition processes by hybrid model based on direct simulation Monte Carlo method"
(ハイブリッドモデルによるクラスター成長・堆積プロセスのマルチスケール計算)

H. Mizuseki, H. Kenta, Y. Kawazoe, L. T. Wille,
**Comput. Mater. Sci** 24, 88-92(2002) [Q1-journal]
DOI: 10.1016/S0927-0256(02)00168-4

* A10; " Hybrid model simulation of the cluster deposition process"
(クラスター堆積プロセスのハイブリッドモデル計算)

K. Hongo, H. Mizuseki, Y. Kawazoe, L. T. Wille,
**J. Cryst. Growth.** 236, 429-433(2002) [Q2-journal]
DOI: 10.1016/S0022-0248(01)02106-6

* A09; " Multiscale simulation of cluster growth and deposition processes by direct simulation Monte Carlo method"
(直接計算モンテカルロ法によるクラスター成長・堆積プロセスのマルチスケール計算)

H. Mizuseki, H. Kenta, Y. Kawazoe, L. T. Wille,
**Scr. Mater.** 44, 1911-1914(2001) [Q1-journal]
DOI: 10.1016/S1359-6462(01)00807-7

* A08; "A Monte Carlo simulation on the process of cluster deposition"
(クラスター堆積プロセスのモンテカルロ計算)

K. Hongo, H. Mizuseki, Y. Kawazoe,
**Mater. Trans.** 42, 439-442(2001) [Q3-journal]
DOI : 10.2320/matertrans.42.439

* A07; "Detecting Complex Orbital Ordering"
(複素軌道状態の観測可能性)

R. Maezono,
**Phys. met. metallogr** 91, S172-S173 (2001) [Q2-journal]

* A06; "Complex orbital state in manganites"
(マンガン酸化物における複素軌道状態)

R. Maezono and N. Nagaosa,
**Phys. Rev. B** 62, 11576 (2000) [Q1-journal]
DOI : 10.1103/PhysRevB.62.11576

* A05; "Spin and orbital ordering in double-layered manganites"
(層状マンガン酸化物のスピン・軌道秩序)

R. Maezono and N. Nagaosa,
**Phys. Rev. B** 61, 1825 (2000) [Q1-journal]

DOI : 10.1103/PhysRevB.61.1825

* A04; "Theory of spin wave excitation in manganites"
(マンガン酸化物におけるスピン波励起)

R. Maezono and N. Nagaosa,
**Phys. Rev. B** 61, 1189 (2000) [Q1-journal]
DOI : 10.1103/PhysRevB.61.1189

* A03; "Role of Orbitals in Manganese Oxides - Ordering and Fluctuation"
(マンガン酸化物における軌道自由度)

R. Maezono, S. Murakami, N. Nagaosa, S. Ishihara, M. Yamanaka, and H.C. Lee,
**Mat. Sci. Eng. B** 63, 171 (1999) [Q2-journal]
DOI : 10.1016/S0921-5107(99)00069-0

* A02; "Phase diagram of manganese oxides "
(マンガン酸化物の相図)

R. Maezono, S. Ishihara, and N. Nagaosa,
**Phys. Rev. B** 58, 11583 (1998) [Q1-journal]
DOI : 10.1103/PhysRevB.58.11583

* A01; "Orbital polarization in manganese oxides "
(マンガン酸化物における軌道偏極)

R. Maezono, S. Ishihara, and N. Nagaosa,
**Phys. Rev. B** (Rapid Communications) 57, R13993 (1998) [Q1-journal]
DOI : 10.1103/PhysRevB.57.R13993

# 著書など

*J8;「スペック理解から読み解く第一原理電子状態計算の実務理解」

前園涼・市場友宏(学生との共著) 単行本: 220 ページ、森北出版 (2020/09/19)、ISBN-13: 978-4627170315

*J7;「自作 PC クラスタ超入門--ゼロからはじめる並列計算環境の構築と運用」

前園涼(単著) 単行本: 176 ページ、森北出版 (2017/12/14)、ISBN-13: 978-4627818217

*J6; "Practical diffusion Monte Carlo simulations for large noncovalent systems"
(非共有結合分子系の大規模量子拡散モンテカルロ計算)

K. Hongo and R. Maezono, Chapter 9, pp 127-143 (2016), in ACS Books "Recent Progress in Quantum Monte Carlo",
(ACS Symposium Series, Vol. 1234), Shigenori Tanaka, Pierre-Nicholas Roy, Lubos Mitas, eds.,
American Chemical Society.
DOI: 10.1021/bk-2016-1234.ch009

* J5; "A Quantum Monte Carlo Study of the Ground State Chromium Dimer"
(クロム二量体の結合に関する第一原理量子モンテカルロ計算)

K. Hongo and R. Maezono, Chapter 8, pp 91-99 (2012),
in ACS monograph "Advances in Quantum Monte Carlo", (ACS Symposium Series, Vol. 1094),
Shigenori Tanaka, Stuart M. Rothstein, William A. Lester , Jr., eds. (ISBN13; 9780841227507),
American Chemical Society.

* J4;「量子モンテカルロ法による多体波動関数理論の展開」

前園涼、§I.2.3, pp.49-65, (2011)
赤井久純、白井光雲編「密度汎関数理論の発展とマテリアルデザインへの応用」
シュプリンガージャパン/丸善・分担執筆.

* J3;「量子モンテカルロ法による電子状態計算の実用化」

前園涼、§4.5, pp.212-218 (2009).
日本計算工学会編「計算力学シミュレーションハンドブック・超ペタスケール
コンピューティングの描像」ISBN-10: 4621082159（丸善・分担執筆）

* J2; "Ab Initio Biomolecular Calculations Using Quantum Monte Carlo combined with the Fragment Molecular Orbital Method"
(量子モンテカルロ法を用いたフラグメント分子軌道法)

R. Maezono, Hirofumi Watanabe, Shigenori Tanaka
Symposium Series No.953/Advances in Quantum Monte Carlo,
J.B. Anderson and S.M. Rothstein eds. (ISBN;9780841274167)
Chapter10, pp. 141-146 (2006), American Chemical Society.

* J1; "MCQMC Study on Positronic Compounds"
(多成分量子モンテカルロ法によるポジトロニウム化合物の計算)

Y. Kita, R. Maezono, and M. Tachikawa,
Lecture Series on Computer and Computational Scieces, "Recent Progress in Computational Sciences and Engineering",
Theodore Simos and George Marioulis eds.,
volume 7, pp.260-263 (2006).
Koninklijke Brill NV, Leiden, The Natherlands.

# 総説など

* D6;「計算科学プログラムはどんどん読みづらくなる–拡散モンテカルロ法電子状態計算の展開に見る近年のトレンド」、前園 涼、

月刊『化学』Vol.74(March.2019)/シリーズ記事「2019 年の化学:最新のトピックス」、化学同人

* D5;「新結晶・新物質 正方格子をもつ新超伝導体 BaTi2Pn2O (Pn = Sb, Bi)」、矢島 健, 中野 晃佑, 陰山 洋、

固体物理 48 (2), 75-82 (2013), アグネ技術センター.

* D4;「ソフト紹介；XCrySDen」、前園 涼、

トラ技ジュニア 12 月 10 日号(2013)、CQ 出版(株)

* D3; "Precise ab-initio calculations of Nano Materials" (in Japanese)

Ryo Maezono,
Review article appeared in The Bulletin of the Society of Nano Science and Technology, 3 87-95 (2005) .
「ナノ・クラスタ科学における精密電子状態計算」
前園 涼,
ナノ学会会報第 3 巻 2 号 87-95 (2005)、ナノ学会.

* D2; "First-Principles Quantum Monte Carlo methods" (in Japanese)

Ryo Maezono,
Review article appeared in'Kotai Butsuri' 39 779-790 (2004) (AGNE GIJUTSU CENTER).
「量子モンテカルロ法による第一原理計算法」
前園 涼,
固体物理 39 779-790 (2004)、アグネ技術センター.

* D1; "First-principles study with Diffusion Monte Carlo code"

Ryo Maezono
Invited paper appeared in 'Activity Report 2002' for Materials Design and Characterization Laboratory, Institute for Solid State Physics, University of Tokyo.
（東京大学物性研究所）